

## COMPUTATIONAL FLUID DYNAMICS MODELING OF SPONTANEOUS HEATING IN LONGWALL GOB AREAS

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### Abstract

In order to provide insights for the optimization of ventilation systems for U. S. underground coal mines facing both methane control and spontaneous combustion issues, a computational fluid dynamics (CFD) study was conducted to model the potential for spontaneous heating in longwall gob areas. A two longwall panel district using a bleeder ventilation system was simulated. The permeability and porosity profiles for the longwall gob were generated from a geotechnical model and were used as inputs for the CFD modeling. In this study the effect of methane emissions from the mined coal seam, including the longwall face and overlying rider seam reservoirs on the gob gas distribution was considered. The spontaneous heating is modeled as the low-temperature oxidation of coal in the gob using kinetic data obtained from previous laboratory-scale spontaneous combustion studies. Unsteady state simulations were conducted and the effects of the coal's apparent activation energy and reaction surface area on the spontaneous heating process were also examined.

Disclaimer: The findings and conclusions in this report are those of the authors and do not necessarily represent the views of the National Institute for Occupational Safety and Health.

### Introduction

In the United States, approximately 17% of the 87 total reported fires for underground coal mines for the period 1990 – 1999 were caused by spontaneous combustion [1]. The risk of an explosion ignited by a spontaneous combustion fire was also present in those mines with appreciable levels of accumulated methane. In fact, three of the mine fires from the reported period resulted in subsequent methane explosions. The incidence of such fires and resulting explosion hazard is expected to increase with the projected increased mining of lower rank coals, deeper mines (more methane), and the growth in the dimensions of longwall panels (ventilation strain).

Spontaneous combustion occurs when the heat that is produced by the low temperature reaction of coal with oxygen is not adequately dissipated by conduction or convection, resulting in a net temperature increase in the coal mass. Under conditions that favor a high heating rate, the coal attains thermal runaway and a fire ensues. The spontaneous combustion potential of coals can be evaluated qualitatively in a laboratory using one of four commonly used methods: adiabatic calorimetry, isothermal calorimetry, oxygen sorption, and temperature differential methods. Although laboratory results are valuable, their extrapolation to the mining environment has not been completely successful because of complicated scaling effects that cannot be reproduced in small-scale experiments. In actual spontaneous heating events in coal mines, much larger coal masses may be involved. The spontaneous heating of coal in mines often occurs in a gob area and is not easily detected. The amount of coal that accumulates in these areas and the degree of ventilation can combine to give optimum conditions for spontaneous combustion. Although much research has been done in experimental study and mathematical modeling of spontaneous combustion of coals [2-11], most of the research was mainly focused on small size coal stockpiles. Saghafi et al. did numerical modeling of spontaneous combustion in underground coal mines with a back return U-ventilation system [12, 13], but their work was limited to two dimensions. Balusu et al. conducted a CFD study of gob gas flow mechanics to develop gas and

spontaneous combustion control strategies for a highly gassy mine [14].

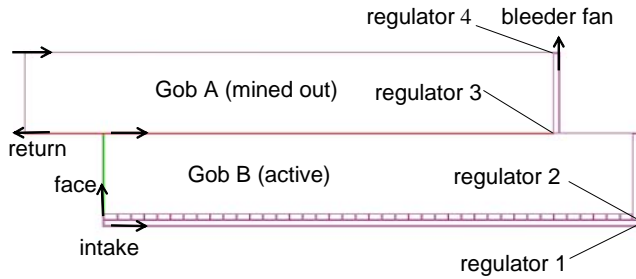
In order to prevent the occurrence of spontaneous combustion in a gob area, it is important to investigate the spontaneous heating of coals under realistic mine ventilation conditions with realistic methane generation and coal chemistry. In previous research carried out by NIOSH, computational fluid dynamics (CFD) modeling was used to describe the ventilation pathways through the immediate gob under different ventilation schemes, and the possible location of critical velocity zones where the gob is most liable to spontaneous heating was discussed [15]. In this paper, preliminary three-dimensional CFD modeling of spontaneous heating of coals in a two-panel gob area using a bleeder ventilation system is presented.

### Gob Layout and Ventilation System

A typical longwall district in an underground coal mine may consist of multiple panels. These panels are typically ventilated using bleeder fans to ventilate the active and mined-out panels. In coal seams with a high spontaneous combustion potential, bleederless ventilation systems are frequently employed. In this work, this situation is simulated with two panels, one as a mine-out panel and the other one as an active panel, utilizing a bleeder system and a bleeder fan. The layout of the two panels and the ventilation system is shown in Figure 1. Each simulated gob area is 2,000 m long, 300 m wide, and 10 m high starting from the bottom of the coal seam. The ventilation airways are 2 m high and 5 m wide. Panel A represents the completed panel, while panel B represents the active one. The ventilation scheme includes a three-entry bleeder system. This scheme and the panel dimensions are typical of longwall mines operating in the Northern Appalachian Coal Basin of the Pittsburgh coal seam. In the model, it is assumed that the middle entry between panel A and B and an entry on panel A's tailgate side are partially open. All crosscuts between the first and second entries on the tailgate side of panel B are open. The bleeder entries at the back end of the gob are represented as one entry connecting to the bleeder fan for modeling purposes. Four regulators are located at the end of the second and third intake entries and two tailgate entries, respectively, for controlling the bleeder ventilation. Major assumptions used to construct the model are summarized as follows:

- (1) Gobs A and B are modeled as two porous rectangular volumes, each with dimensions of 2000 m × 300 m × 10 m.
- (2) Gobs A and B have the same permeability and porosity distributions. The permeability and porosity varies with the panel length and width, but not the height.
- (3) Between panels A and B, only the middle entry is open and is characterized by the porosity and permeability values. Crosscuts on panel B tailgates and panel A headgate are assumed crushed into the gob areas.
- (4) Right above the middle entry between the panel A and panel B is the original rock with certain porosity and permeability values.
- (5) The entry at panel A tailgate is modeled the same way as the middle entry between panel A and B. The rock volume right above this entry is not modeled.

- (6) Crosscuts on the B panel headgate are open while crosscuts connecting each panel and bleeder entries at the back end of each panel are closed.



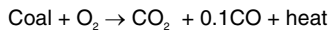
**Figure 1.** Layout of gob areas and ventilation system.

### Low Temperature Coal Oxidation

The chemical reaction between coal and oxygen at low temperatures is complex. Generally, three types of processes are believed to occur [7]. These are: (i) physical adsorption; (ii) chemical adsorption which leads to the formation of coal-oxygen complexes and oxygenated carbon-species; and (iii) oxidation in which the coal and oxygen react with the release of gaseous products, typically carbon monoxide (CO), carbon dioxide (CO<sub>2</sub>), and water vapor (H<sub>2</sub>O).

The moisture content of coal can play an important role in the low temperature coal oxidation. The interaction between water vapor and coal can be exothermic or endothermic depending on whether the water condenses or evaporates. Sondreal and Ellman [16] reported that for dried lignite, the rate of temperature increase due to the adsorption of water increased with the moisture content up to a value of 20 % water (by mass) and then decreased with further increasing moisture content. Smith and Lazzara [5] found that the effect of the moisture content of the air on self-heating process was also dependent on coal rank and temperature.

During the first stage of this study, the effect of water vapor is not considered, and the chemical reaction between coal and oxygen is simplified as:



The detailed chemical structure of coal is not clear and varies with the rank and origin of coal. According to experimental data [5], one mole of coal reacting with one mole of oxygen generates one mole carbon dioxide and roughly 0.1 mole carbon monoxide plus heat at the early stage of coal oxidation. The dependence of the rate of oxidation on temperature and oxygen concentration can be expressed in the form:

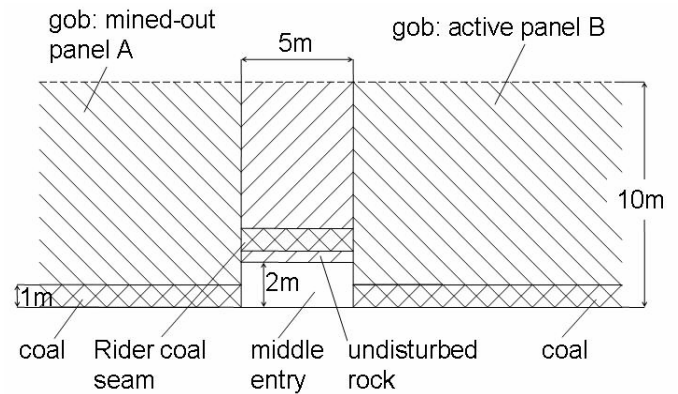
$$\text{Rate} = A[\text{O}_2]^n \exp(-E/RT)$$

where the chemical reaction rate is defined as the rate of change in the concentrations of the reactants and products, A is the preexponential factor, E is the apparent activation energy that is the energy needed to initiate a chemical reaction, R is gas constant, n is the apparent order of reaction, T is the absolute temperature and [O<sub>2</sub>] is the oxygen concentration.

The value of apparent activation energy, E, of different coals can vary between 12 and 95 kJ/mol. It is about 90 kJ/mol for Pittsburgh coal, which is considered to have a moderate potential to spontaneous heating [5, 17]. The pre-exponential factor, A, depends more on coal rank and measurement method, and has a typical value between 1 and 7×10<sup>5</sup> /s. The value of the apparent order of the reaction, n, in low-temperature oxidation studies of coal and other carbonaceous materials has been shown to vary from ~0.5 to 1.0 [5, 7], and is about 0.61 for some U.S. coals [2]. The heat of reaction of coal oxidation is approximately 300 kJ/mol-O<sub>2</sub> for Pittsburgh coal.

In order to simulate the spontaneous heating of coal in longwall gob areas, the source of coal needs to be defined. The coal source can be coal left from the mined coal seam or other overlying or

underlying coal seams. In this study, the Pittsburgh coal seam was considered with a 1-meter thick rider coal seam less than 1 m above the 2-meter thick main coal seam. The rider seam was modeled as caving into the gob after the main coal seam was completely mined out. Figure 2 shows the cross section of two longwall panels with the caving coal layer at the bottom of the gobs. The coal pillars left along the perimeter of the gob were also considered as a coal source. The oxidation of coal will occur on any available coal surface including both external and internal pore surfaces. The reaction rate of spontaneous heating of coal in coal stockpiles was found to be related to the external surface area for nonporous coal particles with small pore diameters, and weakly related or not related to particle size for small porous coal particles with larger pore diameters [7]. It is difficult to define a coal particle size distribution in the coal layer in the gob area because of the large gob size. The parameter that affects the heat generation and dissipation during the spontaneous heating process is the coal surface area available in a unit volume, or surface-to-volume ratio. If an average coal particle diameter of 5 cm is assumed, then the surface-to-volume ratio would be 72 /m using a typical porosity value of 0.4 within the uncompacted gob. The heat generated from oxidation will be dissipated by conduction and convection while the oxygen and oxidation products are transported by convection and diffusion.



**Figure 2.** Cross section of two longwall panels with caving coal layer.

### Estimation of Gob Permeability

The permeability and porosity distributions of the gob areas were based on geotechnical modeling of longwall mining and the associated stress-strain changes using FLAC<sup>1</sup> (Fast Lagrangian Analysis of Continua) code [18]. In FLAC modeling, mining was simulated in increments, starting from one side of the grid and advancing to the other side. Extraction of the coalbed was modeled by removing elements over the height of the coalbed. The process of gob formation was modeled by first deleting rock elements in the roof of the coalbed, so that they are stress relieved, followed by inserting gob properties in these elements. Gob properties were also inserted in previously mined coalbed elements, so that the gob filled the mined void. In the gob caved area, the re-compaction of the caved rock has a significant effect on its permeability. Stress changes in the rock in the gob cause changes in the fracture apertures which then impact the permeability. Immediately behind the advancing face, the caved rock is loosely stacked and has an estimated porosity of approximately 0.4. As the mining face advances away from this caved rock, the weight of the overburden gradually increases and re-compacts the caved rock. This loading or stress in the caved material increases exponentially, until the full overburden load is supported by the caved material. The re-compaction, estimated with the FLAC model's assigned strength and mechanical properties of the gob material, results in a reduction in the void space within the broken rock rubble and, therefore, significant changes in permeability. A simple relationship was used to estimate the changes in permeability in the caved rock based on the Kozeny-Carman equation:

<sup>1</sup> Reference to a specific product is for informational purposes and does not imply endorsement by NIOSH.

$$k = f \left( \frac{n^3}{(1-n)^2} \right)$$

where  $n$  is the porosity and  $k$  is the permeability.

For a Pittsburgh coal seam longwall panel, the permeability values in the gob area were estimated to vary from  $3.0 \times 10^4$  to  $8.5 \times 10^5$  millidarcies (md), while the porosity value varies from 0.17 to 0.41. Around the perimeter of the gob and immediately behind the face shields, the permeability and porosity values were the largest, while near the center of the gob, these values were the smallest due to compaction. A detailed description of permeability calculation is given in Esterhuizen and Karacan [19]. These permeability and porosity distributions were then used in FLUENT as input.

Figure 3 shows the permeability variation with the panel length and width for panel A. The same profile was also applied to panel B. The porosity profiles in the two panels were similar to those permeability profiles except the maximum and minimum values are 0.41 and 0.17, respectively. It is assumed that these permeability and porosity files do not change with the gob height

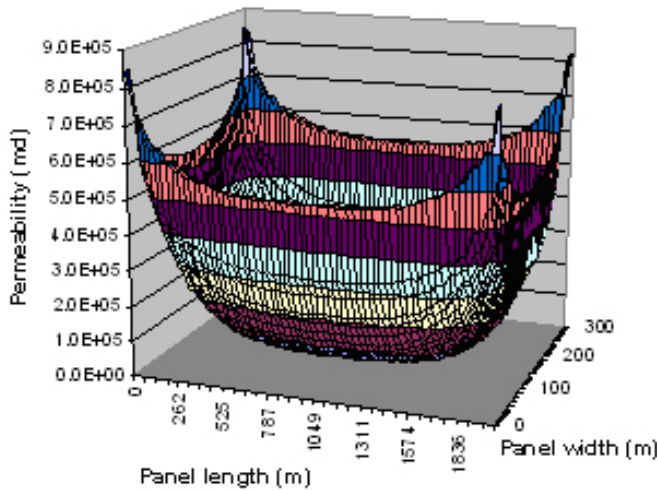


Figure 3. Permeability distributions for the gob.

#### Numerical Modeling

A commercial CFD software, FLUENT from Fluent, Inc., was used in this study to simulate the gas flow and spontaneous heating in the longwall gob areas. The gas flow in the longwall mine gob area was treated as laminar flow in a porous media using Darcy's law, while the gas flow in the ventilation airways was simulated as fully developed turbulent flow. The physical model and mesh for the CFD simulation were generated using the mesh generator software, GAMBIT, from Fluent, Inc. The cell size varies from 1 to 4 m in the model with larger size cells located near the center of the gob. The total cell number was over 1.5 million.

Methane emission was also considered in the simulation because it affects the oxygen concentration distribution in the gob. Methane is always liberated from the face and inside the gob from the coal remaining within and around the gob. Under normal mining conditions, most of the methane from the gob coal is released in the first several hours, after which the release becomes very slow [20]. Since the time period for spontaneous combustion is typically at least several days, the gob coal methane emission is not considered in this simulation. Another source of continuous gob methane emission is from any overlying rider coal seam reservoirs. The methane from the overlying coal seam reservoir is assumed to be released uniformly along the border between the gob and the reservoir. Using ventilation data from a local Pittsburgh coal seam mine, the amount of methane released from the reservoir in this simulation is 281 cfm for panel B and 50 cfm for panel A. The methane emission rate from the face to the panel B is

29 cfm. These data were also entered into FLUENT using C subroutines.

The boundary conditions for ventilation pressures used in the simulation were also obtained from a local Pittsburgh coal seam mine's ventilation data. The pressure was -3.0 inches water gauge at the intake inlet, -3.5 inches water gauge at the return outlet, and -11.0 inches water gauge at the bottom of the bleeder shaft. The wall roughness of the ventilation airways was adjusted to have a total intake airflow rate of 87,000 cfm in the active longwall panel. The pressure drops through the two regulators located at the second and third intake entries were also adjusted to have an airflow rate entering onto the face of 60,000 cfm. The pressure drop at regulator 3 was adjusted to have a flow rate at the return of 50,000 cfm, and the flow rate in the entry on panel A's tailgate side was 7,000 cfm by adjusting the pressure drop at the regulator 4.

A simulation was conducted first without coal oxidation to obtain steady state flow field and gas distributions. Then, the unsteady simulation with coal oxidation was conducted using the steady state solution as the initial conditions. The face was assumed stationary during the simulation. The physical and kinetic properties of the coal layer are listed in Table 1. The kinetic properties of coal oxidation were obtained from the previous laboratory-scale spontaneous combustion studies conducted by Smith and Lazzara [5].

Table 1. The physical and kinetic properties of the coal layer.

Coal density	1300	kg/m <sup>3</sup>
Coal specific heat	1003.2	J/kg-K
Coal conductivity	0.1998	W/m-K
Heat of reaction	300	kJ/mol-O <sub>2</sub>
Activation energy	89.9	kJ/mol
Pre-exponential factor	$6 \times 10^4$	/s
Porosity	0.4	-
Initial coal temperature	300	K

#### Flow Patterns inside the Gob

CFD The flow patterns inside a gob will have a significant effect on the spontaneous heating of coals because the oxygen needed for the oxidation is provided by the gas flow, and the heat generated from the oxidation may be carried away by the gas flow. The gas flow inside a gob is expected to be three dimensional with the flow in the vertical direction, but weaker than in the other two directions due to reduced permeability and pressure gradients. In order to visualize the flow patterns inside the gob, a virtual horizontal reference surface was created 1 m from the bottom of the mined seam floor to compare the results with respect to this horizontal reference surface. Figure 4 shows the steady state pressure distribution over the two gob areas. A pressure differential was established between the intake and return, and between the face and the bleeder fan with higher pressure at the face and lower pressure at the bleeder fan. Figure 5 shows the flow path lines colored by velocity magnitude in the two gob areas. The path lines indicate that the flow was mainly from the headgate side to the tailgate side in the two panels. At the face, air entered into the gob through the face shields and flowed to the middle entry between the two panels. The higher gas velocity was between  $1.5 \times 10^{-4}$  to  $2.5 \times 10^{-4}$  m/s (0.03 to 0.05 fpm) near the back end of panel B.

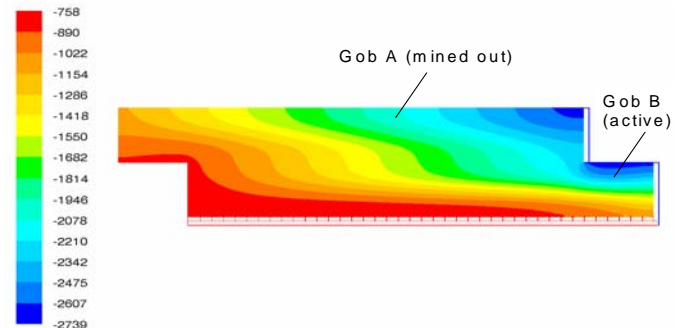
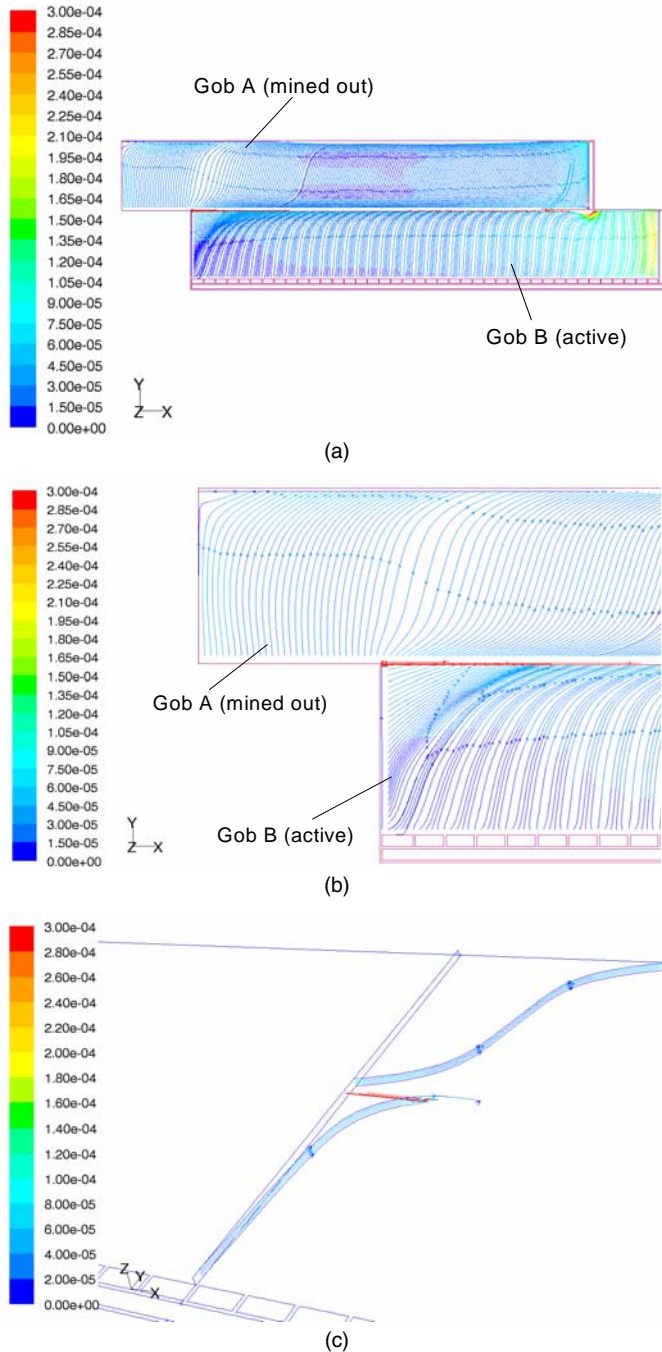


Figure 4. Contours of static pressure (pascal) over gob areas.





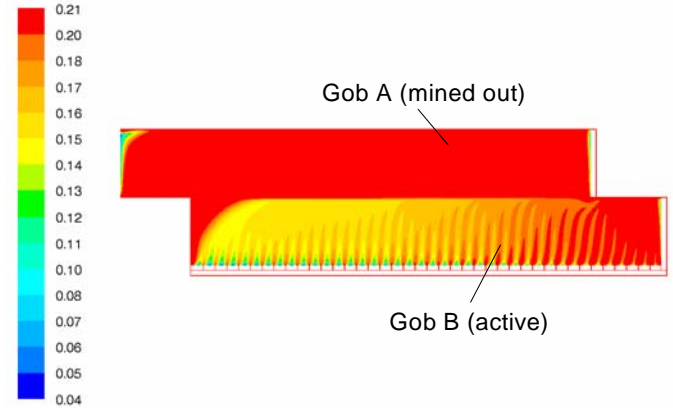
**Figure 5.** Flow path lines colored by velocity magnitude (m/s) in gob areas: (a) over the entire gob areas; (b) near the face area; (c) in a vertical cross section 1000 m from the face.

Figure 6 shows the oxygen distribution in two panels. The oxygen concentration was at 21% in most of mined-out gob A. In the active gob, B, the oxygen concentration close to the intake entry was below 21% because of methane emission from the overlying coal seam reservoir. The opening of crosscuts between the first and second intake entries appears to be very important to dilute the methane concentration near the perimeter of the gob on the headgate side of the active panel.

### Simulation Results and Discussion

Simulations of spontaneous heating of coals were conducted with different values of apparent activation energy and coal surface area to investigate the effects of activation energy and coal surface area on

the spontaneous heating of coal in gob areas as shown in Table 2. Case 1 represents a typical Pittsburgh coal seam, while case 2 represents a coal with lower rank values typical of a Western coal. Case 3 represents the Western coal with a lower surface-to-volume ratio. The pre-exponential factor A was kept the same,  $6 \times 10^4$  /s, for the three cases.



**Figure 6.** Contours of oxygen concentration (1=100%) in gob areas.

**Table 2.** Simulation scenarios.

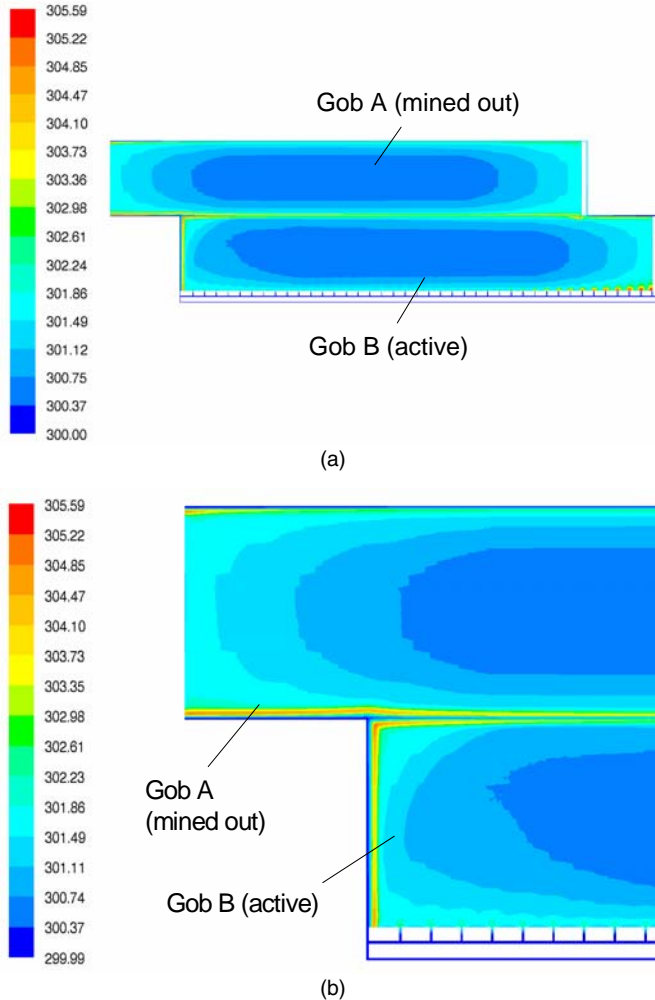
Case	Activation energy (kJ/mol)	Surface-to-volume ratio (/m)
1	89.9	72
2	52.7	72
3	52.7	12

### Effect of Apparent Activation Energy

Figure 7 shows the temperature distribution in the two panels after about 14 days for case 1. The maximum temperature was 305 K (32°C), a 5 degree increase. The maximum temperature increases occurred near the tailgate corner of panel B, in the return split between panel A and B, and just inside the crosscuts near the back of panel B. For case 2, shown in Figure 8, where the coal had a lower activation energy, the maximum temperature was 564 K (291°C), a 264 degree increase, after only 5 days. According to reference [17], when the coal temperature reaches above 503 K (230°C), the spontaneous heating mechanism changes to rapid combustion. So under the conditions of case 2, a fire would likely occur given a sufficient oxygen supply. Case 1 can be viewed as representative of a coal with a moderate self-heating tendency, like Pittsburgh coal. For this kind of coal, the spontaneous combustion hazard is usually moderate under normal mining conditions. Case 2 represents a coal with a high self-heating tendency. For this kind of coal, the spontaneous heating hazard is considered high, according to reference [5] under normal mining conditions. For case 1, although the temperature rise was lower, it was observed over most of the gob except the center area of the gob. In case 2, the much higher temperature rise was limited to some very narrow areas behind the face shields and close to the middle entry between the two panels. In panel A, the temperature rise occurred close to the return airway and the middle entry on its tailgate side. In panel B, the temperature rise occurred on the tailgate side near the back end of the gob and the regulator 3. It is interesting to see that most of the gob area was still at its initial temperature. It should be pointed out that in a real situation similar to case 2, a bleederless ventilation system may be needed instead of a bleeder ventilation system.

The oxygen concentration distributions for two cases are shown in Figure 9. For case 1, oxygen was still available throughout most of the gob and 21% oxygen was available at a short distance behind the shields and close to the middle entry and return airway. Deeper into the gob, oxygen concentration dropped to about 3%. For case 2, there was no oxygen left even immediately behind the shields or close to the middle entry. Deeper into the gob, the oxygen concentration was near zero everywhere, indicating that the oxygen was nearly all consumed by the oxidation of the coal near the active mining face. These oxygen

distributions indicate that spontaneous heating is mainly controlled by oxygen availability when significant temperature rise occurs. This explains why the temperature rise only occurred in the area behind the shields and the area close to the middle entry, because oxygen was only available in these areas. Under the ventilation conditions studied here, not enough oxygen could be carried to the compressed gob area through convection and diffusion.



**Figure 7.** Temperature distribution (K) for case 1 after 14 days: (a) over the entire gob areas; (b) near the face area.

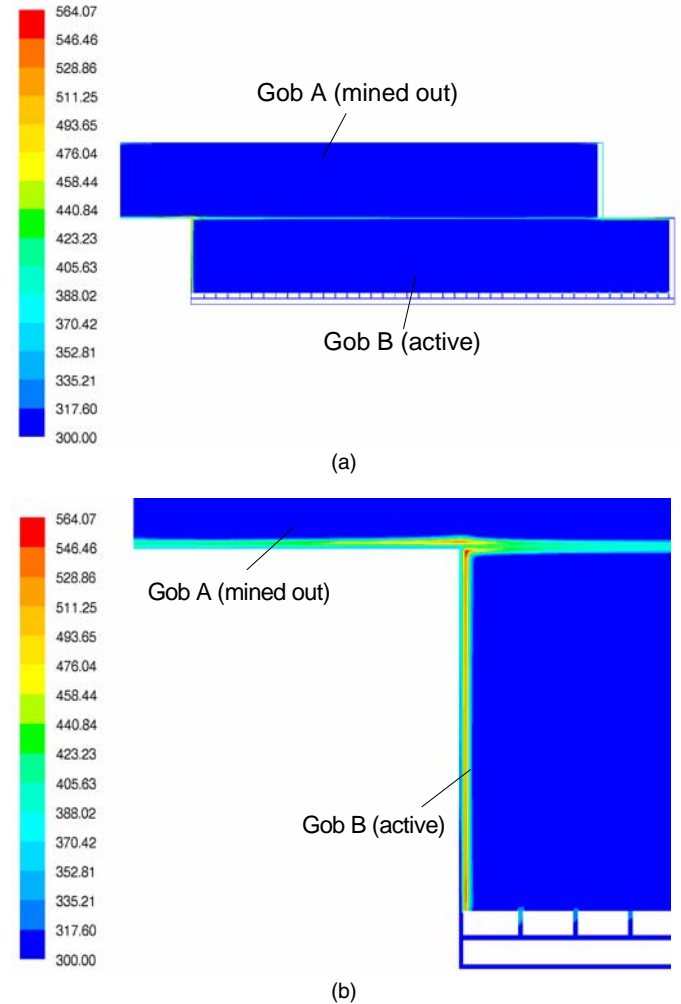
#### Effect of Coal Surface Area

The effect of coal surface area on the spontaneous heating was also examined by using a lower surface-to-volume ratio of 12 /m, equivalent to an average coal particle diameter of 30 cm, and an activation energy of 52.7 kJ/mol, while the other parameters were kept the same as in case 2. Figure 10 shows the temperature distribution over the two panels after 5 days. Compared with Figure 8, the temperature distribution was very similar except that the maximum temperature was 370 K (97 °C), a 70 degree rise. This is much lower than the value for the higher surface-to-volume ratio in case 2, indicating that a larger particle size caused a smaller temperature rise in the same period of time. It was further found that after 25 days, the maximum temperature was 226 °C, still below 230 °C, indicating that decreasing the coal reaction surface area will greatly reduce the spontaneous combustion fire hazard.

#### CO Concentration Distribution

The carbon monoxide concentration distribution for case 3 after 5 days is shown in Figure 11. The maximum CO concentration was 1.7%. The location of the maximum CO concentration was nearly the same areas of the maximum temperature indicating the reaction

products were not transported away quickly. CO is usually used as an indicating gas for spontaneous heating of coals in mine fire detection. Although the maximum CO concentration was 1.7%, it was diluted to about 4000 ppm at the outlet to the bleeder fan by the air from the bleeder entry.



**Figure 8.** Temperature distribution (K) for case 2 after 5 days: (a) over the entire gob areas; (b) near the face area

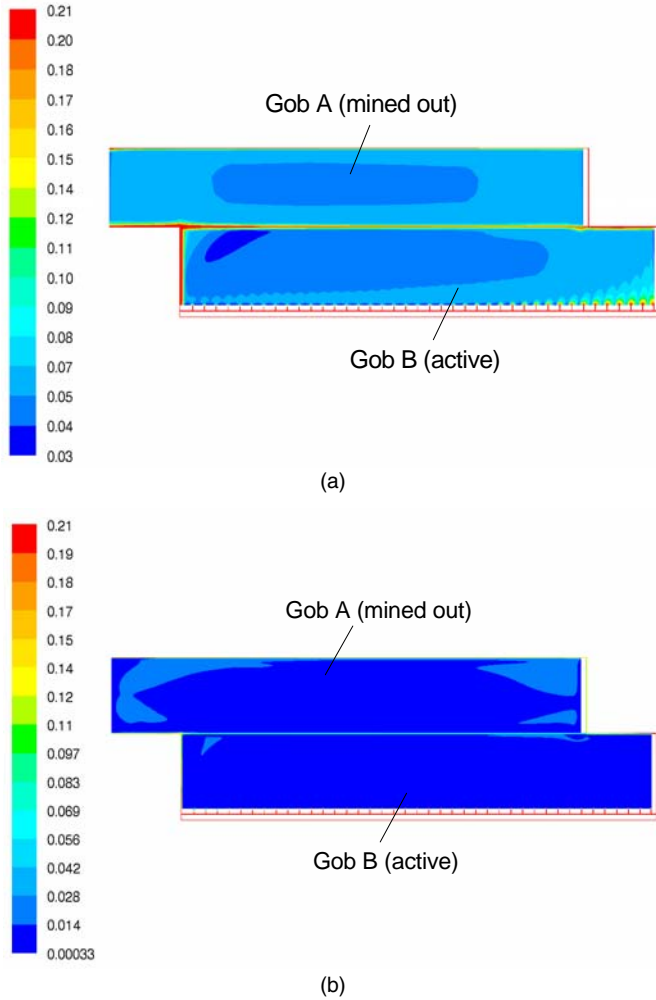
#### Oxygen Concentration near the Top of the Gob

It is also worth to note that some oxygen was still available above the coal layer. Figure 12 shows the oxygen concentration distributions at the horizontal surfaces 1m and 9 m above the bottom of the coal seam, respectively, for case 3. At the 1-meter surface, nearly all oxygen was consumed, while much higher oxygen concentrations existed on the 9-meter surface. The model showed that this oxygen could not be transferred to the oxidation zone through convection and diffusion.

#### Critical Velocity Zones for Spontaneous Combustion

As discussed in reference [15] and shown in this investigation, just behind the shields where the oxygen concentration is highest, the air velocity is also high, so that heat generated by self-heating is carried away. Deeper in the gob, the air velocity is too low to provide sufficient oxygen to support spontaneous combustion. This was confirmed in the simulations. Under conditions studied here, the simulations demonstrate that the area about 5 to 9 meters behind the shields was indeed the critical velocity zone for potential spontaneous combustion. In the active panel B, the critical velocity zones also occurred in the narrow area near the middle entry, and the narrow area on the tailgate side of the panel and near the back end of the gob, and the area near the open crosscuts between the first and second intake

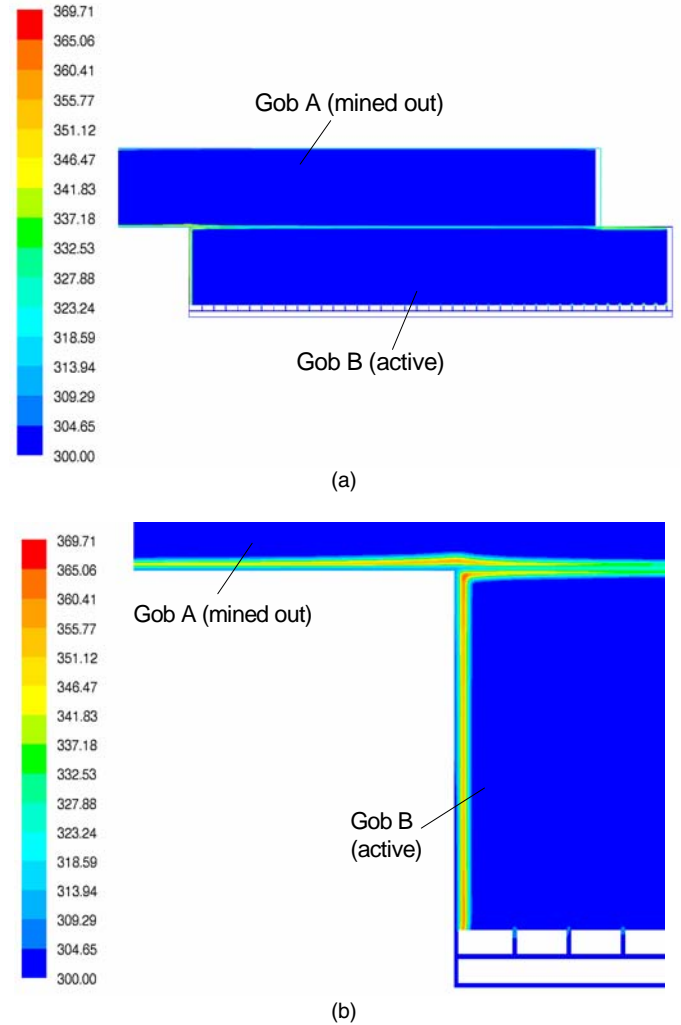
entries. In the mined-out panel A, the critical velocity zone occurred in the narrow area near the return entry, and the narrow area near the middle entry on both headgate and tailgate sides. All these narrow areas were about several meters wide.



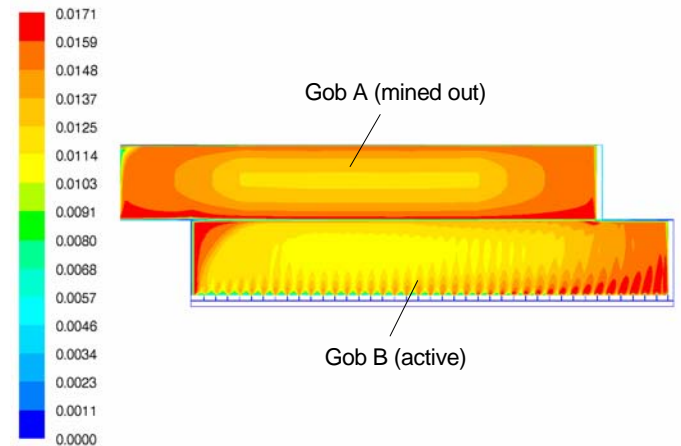
**Figure 9.** Oxygen concentration distribution (1=100%) in two gob areas: (a) case 1; (b) case 2

### Conclusions

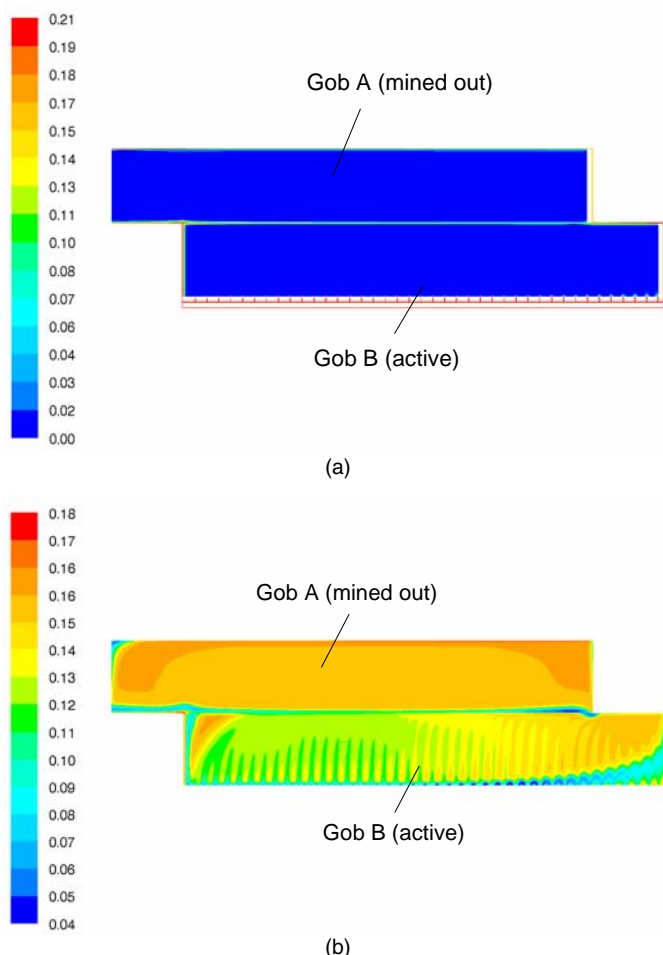
CFD simulations were conducted to investigate the spontaneous heating of coals in longwall gob areas with different apparent activation energies and reaction surface areas. Simulation results demonstrate that under typical three-entry bleeder ventilation conditions, the spontaneous heating hazard was minimal for coals with a higher apparent activation energy for at least two weeks. The hazard was high for coals with lower apparent activation energies after 5 days. When the temperature rise was significant, the spontaneous heating became mainly oxygen controlled. The temperature rise was greatly dependent on the available reaction surface area. For larger coal particle size, the reaction surface area and the maximum temperature rise were both significantly reduced. Simulations also confirmed the existence of a critical velocity zone behind the shields in the gob, and showed the existence of other critical velocity zones in both the active panel and the mined-out panel. More research is needed to study the effect of the longwall face movement on the spontaneous heating of coals in the gob areas, and modeling of bleederless ventilation systems. Because of the complexity of the problem and lack of field data for gob permeability and porosity distribution, the results reported here are valid only for the permeability and porosity data used in this study with the longwall panel setup and ventilation conditions stated in the paper.



**Figure 10.** Temperature distribution (K) in two gobs for case 3: (a) over the entire gob areas; (b) near the face area



**Figure 11.** CO concentration (1=100%) for case 2



**Figure 12.** Oxygen concentration (1=100%) at two horizontal surfaces for case 3: (a) 1-meter horizontal surface; (b) 9-meter horizontal surface

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